3-Bromophenylurea
2989-98-2 | DTXSID70184008

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 256 °C

Global applicability domain: Outside

Local applicability domain index: 2.32e-01

Confidence level: 7.61e-01

Nearest Neighbors from the Training Set

Image not found
N-(4-Bromophenyl)urea
Measured: 260
Predicted: 256

Image not found
1-Phenylurea
Measured: 238
Predicted: 247

Image not found
Diphenylurea
Measured: 262
Predicted: 269

Image not found
1,3-Dipropylurea
Measured: 255
Predicted: 256

Image not found
Urea, N,N'-diethyl (9CI)
Measured: 263
Predicted: 262